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AN ACCURATE METHOD FOR EVALUATING THE OVERLAP TERM IN THE UNRESOLVED REGION

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An Accurate Method for Evaluating the Overlap Term in the Unresolved Region

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ABSTRACT

An accurate and efficient method has been developed for estimating the overlap effect due to the neighboring resonances of the same spin sequence in the unresolved region. In contrast to the previously developed method, the new method is capable of treating practically all energy regions of interest in the fast reactor applications. The Dyson's correlation function is used to account for the proper correlation of levels. In the numerical calculations, the exact Doppler-broadened line-shape function is used. The method has been made economical for routine calculations in the fast reactor applications.

I. INTRODUCTION

Extensive studies on the role of the resonance overlap effect in fast reactor calculations have been described in previous work.[1,2] A rather crude method was proposed for estimating the overlap effect of neighboring resonances of the same sequence in the unresolved energy region. This early method is believed to be reasonably accurate in the energy region where resonances are strongly overlapping. However, it becomes questionable in the relatively low-energy region and for the cases where the "equivalent" potential scattering cross section becomes small. These are the situations that one must face in the analysis of Doppler-effect experiments and of heterogeneity studies for critical assemblies. The significance of the overlap effect on the temperature dependence of the Doppler coefficient under meltdown conditions where the extremely high temperature of the fuel pin may be accompanied by spectrum hardening due to the loss of sodium must also be realized. Under this condition, even the well-separated ^{238}U resonances become strongly overlapping. The accurate estimation of the overlap effect is, therefore, important in fast reactor safety studies. Some preliminary results concerning this problem have been given in previous work.[3] Hence, an accurate estimation of the overlap effect is desirable.

The purpose of this report is to describe a newly developed method for estimating the overlap effect due to resonances of the same spin sequence in the unresolved energy region. Improvement on the earlier method[1,2] has been made in three general areas. First of all, the exact Doppler-broadened line-shape function $\psi(\sigma,x)$ is used instead of the approximate Gaussian form used previously. Secondly, the new method is

made applicable even in the relatively low-energy region and for cases where the equivalent scattering cross sections per absorbing atoms σ_p^{eq} is small. The assumption that $[\psi(\theta,x)/\beta] << 1$ used in the previous method has been avoided. This assumption obviously breaks down whenever $[\psi(\theta,0)/\beta] \leq 0$. Finally, the Dyson's correlation function[4] for levels is used instead of the rather crude approximation used in the previous work.[1,2] The use of the approximate correlation function described previously was found to underestimate the overlap effect in the high-energy region.[5]

The analytical and numerical foundations of the proposed method are described in detail from Section II through Section V. In order to test and evaluate the merits of the proposed method, a code has been developed. Section VI describes the CHOPSUEY code and its computing time required for calculations of practical interest. The listing of relevant subroutines are also given.

II. FORMULATION OF THE OVERLAP TERM

If the NR-approximation and the "nearest neighbor" approximation[1,2] are assumed, the overlap term for a given process x due to the resonances of the same sequence can be written as

$$\tilde{0}_x = \frac{1}{\langle D \rangle} \left\langle \frac{\Gamma_{xk}}{2} \int_{-\infty}^{\infty} \Omega(\delta) \frac{d\delta}{\langle D \rangle} \int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k} \, \frac{A_{k'}\psi_{k'} \, dx_k}{\beta_k + \psi_k + A_{k'}\psi_{k'}} \right\rangle_{k \text{ and } k'} , \quad (1)$$

where $A_{k'}$ is the ratio of the peak cross section of resonance k´ with respect to a given resonance k and $\langle D \rangle$ is the average level spacing.

made applicable even in the relatively low-energy region and for cases where the equivalent scattering cross sections per absorbing atom σ_e^m is small. The assumption that $[\psi(\theta,x)/S] \sim 1$ used in the previous method has been avoided. This assumption obviously breaks down whenever $[\psi(\theta,0)/S] \leq 0$. Finally, the Dyson's correlation function[4] for levels is used instead of the rather crude approximation used in the previous work.[1,2] The use of the approximate correlation function described previously was found to underestimate the overlap effect in the high-energy region.[5]

The analytical and numerical foundations of the proposed method are described in detail from Section II through Section V. In order to test and evaluate the merits of the proposed method, a code has been developed. Section VI describes the CROSSECT code and its computing time required for calculations of practical interest. The listing of relevant subroutines are also given.

II. FORMULATION OF THE OVERLAP TERM

If the NR-approximation and the "nearest neighbor" approximation[1,2] are assumed, the overlap term for a given process x due to the resonances of the same sequence can be written as

$$O_s = \frac{1}{\langle D\rangle}\left\langle \frac{\pi R}{2}\int_{-\infty}^{\infty}\frac{dE}{\langle D\rangle}\,R(E)\int_{-\infty}^{\infty}\text{[illegible]}\right\rangle_{i\ \text{and}\ k'} \quad (17)$$

where $\lambda_{k'}$ is the ratio of the peak cross section of resonance k' with respect to a given resonance k and $\langle D\rangle$ is the average level spacing.

The brackets $\langle\,\rangle$ indicate the statistical average over the distribution functions of the resonance parameters of both k-*th* and k′-*th* resonances. The correlation function $\Omega(\delta)$ is the probability that any k′-*th* resonance will be found at a distance of $\delta = E_k - E_{k'}$ from a given resonance k. For our purpose, $\Omega(\delta)$ is taken to be Dyson's two-level correlation function.[4,5]

$$\Omega(y) = 1 - \{s(y)\}^2 + \frac{\partial s(y)}{dy}\,si(y)\ , \tag{2}$$

where

$$y = \frac{\pi|E_k - E_{k'}|}{D} \tag{3}$$

$$s(y) = \frac{\sin|y|}{y} \tag{4}$$

and the sine integral si(y) is defined as

$$si(y) = -\int_y^\infty \frac{\sin t}{t}\,dt\ . \tag{5}$$

Equation (1) involves multiple integrals. A direct numerical approach is believed to be extremely time-consuming, if at all practical, for routine design calculations. Equation (1) can be simplified considerably by series expansion.

Note that the integral can be expressed as

$$\int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k}\,\frac{A_{k'}\psi_{k'}}{\beta_k + \psi_k + A_{k'}\psi_{k'}}\,dx_k = \int_{-\infty}^{\infty} \frac{\psi_k}{\beta_k + \psi_k}\left\{\frac{\psi_{k'}}{\beta_{k'} + \psi_{k'}} - \frac{A_k\psi_k\psi_{k'}}{\left(\beta_{k'} + \psi_{k'}\right)^2} + \cdots \right. \tag{6}$$

provided the resulting integrals are uniformly convergent. The substitution of Eq. (6) into Eq. (1) gives

$$\tilde{0}_x = K_1 - K_2 + \cdot\cdot\cdot , \tag{7}$$

where

$$K_1 = \frac{1}{\langle D\rangle^2}\left\langle\Gamma_{xk}J\right\rangle_k\left\langle\Gamma_{k'}J\right\rangle_{k'} - L_1 , \tag{8}$$

$$L_1 = \frac{1}{\langle D\rangle}\int_{-\infty}^{\infty} W\left(\frac{\delta}{\langle D\rangle}\right)\frac{d\delta}{\langle D\rangle}\int_{-\infty}^{\infty}\left\langle\frac{\Gamma_{xk}}{2}\,\frac{\psi_k}{\beta_k+\psi_k}\right\rangle_k\left\langle\frac{\Gamma_{k'}}{2}\,\frac{\psi_{k'}}{\beta_{k'}+\psi_{k'}}\right\rangle_{k'} dx_k , \tag{9}$$

$$J = \int_0^{\infty}\frac{\psi_k\, dx_k}{\beta_k+\psi_k} , \tag{9a}$$

$$K_2 = -\frac{1}{\langle D\rangle^2}\left\langle\tau_{xk}\right\rangle_k\left\langle\frac{\Gamma_{k'}}{2}\,\sigma_p^{eq}\,\frac{\partial}{\partial\sigma_p^{eq}}\,J\right\rangle_{k'} - L_2 , \tag{10}$$

$$L_2 = -\frac{1}{\langle D\rangle}\int_{-\infty}^{\infty} W\left(\frac{\delta}{\langle D\rangle}\right)\frac{d\delta}{\langle D\rangle}\int_{-\infty}^{\infty}\left\langle\frac{\Gamma_{xk}}{2}\left[\frac{\psi_k}{\beta_k}-\frac{\psi_k}{\beta_k+\psi_k}\right]\right\rangle_k\left\langle\frac{\Gamma_k}{2}\,\sigma_p^{eq}\,\frac{\partial}{\partial\sigma_p^{eq}}\,\frac{\psi_{k'}}{\beta_{k'}+\psi_{k'}}\right\rangle_k dx_k , \tag{11}$$

$$\tau_{xk} = \frac{\Gamma_{xk}}{2\beta_k}\int_{-\infty}^{\infty}\frac{\psi_k^2}{\beta_k+\psi_k}\,dx_k = \frac{\pi}{2}\left\langle\frac{\Gamma_{xk}}{\beta_k}\right\rangle - \left\langle\Gamma_{xk}J\right\rangle_k , \tag{12}$$

$$-\frac{\partial}{\partial\sigma_p^{eq}}\left(\frac{\psi_k}{\beta_k+\psi_k}\right) = \left[\frac{\psi_k}{\beta_k+\psi_k} - \frac{\psi_k^2}{\left(\beta_k+\psi_k\right)^2}\right]\frac{1}{\sigma_p^{eq}}\,, \qquad (13)$$

and

$$W\left(\frac{\delta}{\langle D\rangle}\right) = 1 - \Omega\left(\frac{\delta}{\langle D\rangle}\right) . \qquad (14)$$

For cases of practical interest, the series in Eq. (7) is uniformly convergent on physical grounds. In contrast to the series expansion used in the previous work, it is clear that the terms in Eq. (7) will converge more rapidly even in the relatively low-energy region. In the region where the previous series expansion is valid, Eq. (7) is equivalent to the inclusion of many terms in the previous expression. In the high-energy region, both expressions become identical. The rapidity of convergence of Eq. (7) depends on the degree of the self-shielding effect of the given isotope and the ratio of the average level spacing and the Doppler width in the energy region under consideration. Note that $\left\langle\tau_{xk}\right\rangle$ defined in Eq. (12) represents the degree of self-shielding effect and is proportional to $1 - \bar{s}$ where $\bar{s}$ is the self-shielding factor

$$\left\langle\Gamma_{xk}J\right\rangle \Big/ \left\langle\frac{\Gamma_{xk}\pi}{2}\Big/\beta_k\right\rangle .$$

In fact, for practically all problems of interest in the unresolved region, the self-shielding effect is relatively small and $\left\langle\tau_{xk}\right\rangle$ is generally much smaller than $\left\langle\Gamma_{xk}J\right\rangle_k$. From Eqs. (8), (10), and (13), it is obvious that $K_1 >> K_2$ if the self-shielding effect is relatively weak. A similar argument can be made to show that the higher-order terms are also small. It is generally true that the resonance sequence with large average spacing

will tend to have a stronger self-shielding effect in the low-energy region. It will be shown in a later section that one seldom needs to retain the higher-order terms beyond K_2 and all K_n terms become identically zero when the average spacing $\langle D \rangle$ becomes much larger than the corresponding Doppler width and the average total width.

Since the J-integral and other related integrals can be readily evaluated using the algorithm proposed previously,[6] the main task here is to evaluate the integral L_1. Once L_1 is known, L_2 can be evaluated quite readily as one will see.

III. EVALUATION OF L_1

L_1 defined in Eq. (9) is still too complicated and a direct numerical approach will undoubtedly require excessive computing time. Furthermore, $W(\delta/\langle D \rangle)$ involves oscillatory functions which are highly undesirable for quadrature formulas. The problem can be resolved by the use of the Fourier transform technique.

A. Technique of Fourier Transform

Define a function $P_k(\xi)$ such that

$$P_k(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\psi_k e^{i\xi x_k}}{\beta_k + \psi_k}\, dx_k = \mathbf{F}\left\{\frac{\psi_k}{\beta_k + \psi_k}\right\} . \qquad (15)$$

The Fourier transform of $W(\delta/\langle D \rangle)$, say $\omega(\xi)$, is[4,5]

$$\omega(\xi) = \frac{\langle D\rangle}{\sqrt{2\pi}} \left\{ 1 - \left|\frac{\langle D\rangle \xi}{\pi}\right| + \left|\frac{\langle D\rangle \xi}{2\pi}\right| \ln\left[1 + \left|\frac{\langle D\rangle \xi}{\pi}\right|\right] \right\} ; \quad \left|\frac{\langle D\rangle \xi}{2\pi}\right| \leq 1$$

$$= \frac{\langle D\rangle}{\sqrt{2\pi}} \left\{ -1 + \left|\frac{\langle D\rangle \xi}{2\pi}\right| \ln\left[\frac{|\langle D\rangle \xi/\pi| + 1}{|\langle D\rangle \xi/\pi| - 1}\right] \right\} ; \quad \left|\frac{\langle D\rangle \xi}{2\pi}\right| > 1 . \qquad (16)$$

From the convolution theorem and the Parseval theorem,[7] it can be shown quite readily that

$$L_1 = \frac{1}{2\langle D\rangle^2} \int_{-\infty}^{\infty} \sqrt{2\pi}\, \omega(\xi) \left\langle \Gamma_{xk} P_k\left(\frac{\Gamma_k}{2}\, \xi\right) \right\rangle_k \left\langle \frac{\Gamma_{k'}}{2} P_{k'}\left(\frac{\Gamma_{k'}}{2}\, \xi\right) \right\rangle_{k'} d\xi \ . \qquad (17)$$

Note that the quantities inside the brackets are the statistically averaged values over the appropriate distribution functions of resonance parameters. The same subscript can be used for the two averaged quantities.

It is interesting to note that $P_k(\xi)$ is the unique solution of the following integral equation

$$\beta_k P_k(\xi) + \frac{1}{2} \int_{-\infty}^{\infty} e^{-(\xi - t)^2/\theta_k^2 - |\xi - t|} \, P_k(t)\, dt = \sqrt{\pi/2}\; e^{-\xi^2/\theta_k^2 - |\xi|} \ , \qquad (18)$$

where the function on the right-hand side is simply the Fourier transform of the ψ-function as described in Ref. 8.

Before attempting to solve these integral equations, it is important to realize some analytical characteristics of $P_k\left(\Gamma_k \xi/2\right)$. First of all,

$P_k\left(\Gamma_k\xi/2\right)$ is an even function so that $P_k\left(\Gamma_k\xi/2\right) = P_k\left(-\Gamma_k\xi/2\right)$. Secondly, in the limit of large β_k, $P_k\left(\Gamma_k\xi/2\right)$ approaches asyptotically to

$$P_k\left(\frac{\Gamma_k}{2}\,\xi\right) \cong \sqrt{\pi/2}\,\exp\left(-\,\frac{\Delta^2}{4}\,\xi^2 - \frac{\Gamma_k}{2}\,|\xi|\right)\Bigg/\beta_k\ , \tag{19}$$

where Δ is the Doppler width. Thirdly, in another extreme where Γ_k is large compared to Δ, ψ becomes Lorentzian. As a result, $P_k\left(\Gamma_k\xi/2\right)$ approaches

$$P_k\left(\frac{\Gamma_k}{2}\,\xi\right) \cong \frac{\sqrt{\pi/2}}{\sqrt{\beta_k\left(\beta_k + 1\right)}}\,\exp\left[-\,\frac{\Gamma_k}{2}\sqrt{\frac{\beta_k + 1}{\beta_k}}\,\xi\right]\ , \tag{20}$$

according to Eq. (15). Of particular academic interest is the fact that Eq. (20) yields

$$L_1 = \frac{\pi^2}{4\langle D\rangle^2}\left\langle \Gamma_{xk}\Gamma_{k'}\sqrt{\frac{1}{\beta_k\left(\beta_k + 1\right)}}\,\sqrt{\frac{1}{\beta_{k'}\left(\beta_{k'} + 1\right)}}\,\frac{1}{z}\left\{1 - \exp(-z)\,\frac{\sinh z}{z} - \mathrm{Ei}(-z)\left(\cosh z - \frac{\sinh z}{z}\right)\right\}\right\rangle_{k\&k'}\ , \tag{20a}$$

where $-\,\mathrm{Ei}(-z)$ is the exponential integral, and

$$z = \frac{\pi}{\langle D\rangle}\left[\Gamma_k\sqrt{\frac{\beta_k + 1}{\beta_k}} + \Gamma_{k'}\sqrt{\frac{\beta_{k'} + 1}{\beta_{k'}}}\right]\Bigg/2\ . \tag{20b}$$

It follows that

$$K_1 = \frac{\pi^2}{4\langle D\rangle^2}\left\langle \Gamma_{xk}\sqrt{\frac{1}{\beta_k\left(\beta_k + 1\right)}}\,\Gamma_{k'}\sqrt{\frac{1}{\beta_{k'}\left(\beta_{k'} + 1\right)}}\,\phi_0(z)\right\rangle_{k\&k'} , \qquad (20c)$$

where $\phi_0(z)$ is identical to that derived by Moldauer[9] for the correction term of the fluctuation in the reaction cross section based on a completely different physical argument. This signifies the strong analogy between these overlap correction terms.

The characteristics defined by Eq. (19) and Eq. (20) provide some clues on how $\left\langle \Gamma_{xk}P_k\left(\Gamma_k\xi/2\right)\right\rangle$ and $\left\langle \left(\Gamma_k/2\right)P_k\left(\Gamma_k\xi/2\right)\right\rangle$ vary as functions of ξ. This information is extremely important in the subsequent construction of quadrature formulas.

With proper normalization, Eqs. (17) and (18) can be evaluated quite readily using Gauss-Hermite quadratures. Define a new variable

$$\eta = \alpha\xi , \qquad (21)$$

where α is set to be

$$\alpha = \sqrt{(\langle D\rangle/\pi)^2 + (\Delta^2/2) + \gamma^2}$$

and

$$\gamma = \left\langle \Gamma_k\sqrt{\frac{\beta_k + 1}{\beta_k}}\right\rangle \qquad (22)$$

Equation (17) becomes

$$L_1 = \frac{1}{\alpha}\,\frac{1}{2\langle D\rangle^2}\sum_{i=1}^{N} a_i\sqrt{2\pi}\;\omega\left(\eta_i/\alpha\right)\left\langle \Gamma_{xk} g_2\left(\eta_i\right)P_k\left(\frac{\Gamma_k\eta_i}{2\alpha}\right)\right\rangle$$

$$\cdot\left\langle \frac{\Gamma_k}{2}\, g_2\left(\eta_i\right)P_k\left(\frac{\Gamma_k\eta_i}{2\alpha}\right)\right\rangle g_1\left(\eta_i\right) + R_N\ , \qquad (23)$$

where

$$g_2\left(\eta_i\right) = \exp\left[\frac{\Delta^2\eta_i^2}{4\alpha^2}\right] \qquad (24)$$

$$g_1\left(\eta_i\right) = \exp\left[\left(\frac{\langle D\rangle^2}{\pi^2\alpha^2} + \frac{\gamma^2}{\alpha^2}\right)\eta_i^2\right] \qquad (25)$$

$$a_n = \frac{2^{n-1}n!\,\sqrt{\pi}}{n^2\left[H_{n-1}\left(\eta_n\right)\right]^2} \qquad (25a)$$

$$R_N = \frac{N!\,\sqrt{\pi}}{2^N(2N)!}\,f^{(2N)}(y) \qquad (-\infty < y < \infty) \qquad (25b)$$

and η_i is the i-*th* zero of the Hermite polynomial $H_n(\eta)$ and $f^{(2n)}(y)$ is the 2n-*th* derivatives of the integrand. Here, the purpose of changing the variable is to ensure that the integrand varies slowly as a function of η in order to make the Gauss-Hermite quadrature highly efficient regardless what values of $\langle D\rangle$, Δ, Γ_k, or β_k are. Similarly, the integral in Eq. (18) can be replaced by the Gauss-Hermite quadrature so that the resulting equation assumes a matrix equation of the form

$$\mathbf{AP} = \mathbf{B}\ . \qquad (26)$$

By normalizing each row of the matrix element of **A** to its diagonal element, one has

$$A_{ij} = \frac{a_j}{4\alpha} g_1\left(\eta_j\right) g_2\left(\eta_j\right) \Gamma_k \exp\left[\frac{\Delta^2}{2\alpha^2}\eta_i\eta_j - \frac{\Gamma_k}{2\alpha}\left|\eta_i - \eta_j\right|\right] \Big/ N_0 \qquad \text{for } i \neq j \tag{27}$$

and

$$A_{ij} = 1 \; ; \qquad \text{for } i = j \; , \tag{27a}$$

where

$$N_0 = g_2\left(\eta_i\right) \cdot \left[\beta_k + \frac{a_i\Gamma_k}{4\alpha} \cdot g_3\left(\eta_i\right)\right] \tag{28}$$

$$g_3\left(\eta_i\right) = \left[g_2\left(\eta_i\right)\right]^2 \cdot g_1\left(\eta_i\right) \tag{29}$$

$$B_i = \sqrt{\pi/2}\, \exp\left(-\frac{\Gamma_k}{2}\left|\frac{\eta_i}{\alpha}\right|\right) \Big/ N_0 \; . \tag{30}$$

Hence, the quantities $P_k\left(\Gamma_k\eta_i/2\alpha\right)$ needed for Eq. (23) are just the solution of a system of N equations. An efficient matrix inversion routine is needed for this purpose. The matrix **A** can be further simplified by partition utilizing the symmetric properties of P_k. The detailed discussion will be given in the next section. It should be noted that the normalization of the matrix proposed here is extremely important from a

numerical point of view. This ensures that the coefficients of each linear equation will not have vanishingly small magnitudes simultaneously.

From Eq. (23) and Eq. (18), it is clear that the Gauss-Hermite quadrature is most efficient and accurate when the Doppler width is larger than or comparable to the average spacing and the average total width. On the other hand, the Gauss-Hermite quadrature is less efficient when Δ becomes small. Under the latter condition, $P_k\left(\Gamma_k \xi/2\right)$ approaches the exponential form defined by Eq. (20). From a practical point of view, the proposed quadrature is highly desirable because it yields accurate values for cases with large Doppler width where the relative importance of the overlap effect is high. For the cases with small Doppler width where the overlap effect is less important, the accuracy of the results is less critical. It was found that a 10-point Gauss-Hermite quadrature is sufficient to give accurate results.

Since the matrix inversion of a relatively large matrix is generally time consuming, it is, therefore, desirable to optimize the proposed method to suit the routine application.

IV. ECONOMIZATION

The proposed method can be made more economical in two general areas: (1) in the region where β_k is much larger than $\psi\left(\theta_k, 0\right)$, the matrix inversion can be avoided completely; and (2) in the region where the matrix inversion is necessary the matrix $\mathbf{A}$ can be partitioned into four submatrices of the size $N/2 \times N/2$ where N is chosen to be 10 or any even number. The symmetry properties of $P_k\left(\Gamma_k \eta_i/2\alpha\right)$ can be utilized.

1. Asymptotic Region $\left[\dfrac{\beta_k + \psi\left(\theta_k, 0\right)}{\psi\left(\theta_k, 0\right)} \geq 2.5\right]$

As discussed previously,[6] the quantity $\psi_k / \left(\beta_k + \psi_k\right)$ can be represented by a uniformly convergent series

$$\frac{\psi_k}{\beta_k + \psi_k} = \frac{\psi_k}{\beta_k + \rho} + \frac{\psi_k\left(\rho - \psi_k\right)}{\left(\beta_k + \rho\right)^2} + \cdot \cdot \cdot , \tag{31}$$

where the parameter ρ can be chosen so that the resulting integrals converge rapidly. One way of choosing ρ is to set

$$\rho = \frac{\int_0^\infty \psi_k^2 \, dx}{\int_0^\infty \psi_k \, dx} = \frac{1}{2} \psi\left(\sqrt{2}\, \theta_k, 0\right) . \tag{31a}$$

By substituting Eq. (31a) into Eq. (15), it can be shown quite readily[5,8] that

$$P_k\left(\frac{\Gamma_k}{2} \xi\right) \cong \sqrt{\pi/2} \exp\left[- \frac{\Delta^2}{4} \xi^2 - \frac{\Gamma_k}{2} |\xi|\right] \cdot Q(\xi) \Big/ \left(\beta_k + \rho\right) + \cdot \cdot \cdot , \tag{32}$$

where

$$Q_k(\xi) \quad = \quad 1 + \{\rho - U\}/\left(\beta_k + \rho\right) \tag{33}$$

$$U \;=\; \frac{\theta\sqrt{\pi}}{2\sqrt{2}}\left[\exp\left(\frac{\Delta|\xi|}{2\sqrt{2}} + \frac{\theta}{\sqrt{2}}\right)^2 \mathrm{Erfc}\left(\frac{\Delta|\xi|}{2\sqrt{2}} + \frac{\theta}{\sqrt{2}}\right) + \exp\left(\frac{\Delta^2\xi^2}{8}\right) \mathrm{Erf}\left(\frac{\Delta|\xi|}{2\sqrt{2}}\right)\right] , \tag{33a}$$

and Erfc(x) and Erf(x) are the complementary error function and error function, respectively. These functions along with $\psi(y,0)$ can be evaluated by using the exceedingly efficient rational approximation as suggested by Hastings.[10]

It is interesting to note that Eq. (31a) serves dual purposes. First of all, it implies

$$Q_k(0) \quad = \quad 1 \tag{33b}$$

according to Eq. (33). Secondly, the magnitude of the next higher-order term at $\xi = 0$ assumes a minimum value as readily seen by differentiating with respect to ρ. Since $\omega(\xi)$ defined in Eq. (16) is a rapidly decreasing function of ξ and varies approximately exponentially

$$\omega(\xi) \;\simeq\; \frac{\langle D\rangle}{\sqrt{2\pi}} \exp\left[-\frac{\langle D\rangle}{\pi}|\xi|\right] , \tag{33c}$$

the choice of ρ in Eq. (31a) amounts to minimizing the error involved by ignoring the next higher-order term and maximizing the range of validity of Eq. (32) in evaluating L_1. It was found by numerical experimentation that the validity of Eq. (32) when used in evaluating L_1 can be extended down to

$$\frac{\beta_k + \psi\left(\theta_k,0\right)}{\psi\left(\theta_k,0\right)} \geq 2.5 .$$

Approximately 75% of the s-wave and practically all of the p-wave unresolved resonances of the fissile isotopes belong to the asymptotic region. Since Eq. (32) avoids the use of the matrix inversion routine, it represents a significant saving in computing time especially when the fissile isotopes are considered. For fertile isotopes, the asymptotic region for s-wave resonances is much smaller than that for fissile isotopes even though practically all p-wave resonances still belong to this region. It should be noted that, in the absence of the fission-width distribution, the computing time is generally negligible even if the matrix inversion method is used for all mesh points.

2. Non-asymptotic Region

Outside the asymptotic region, accurate calculations can be made by using the matrix inversion technique. Since all quantities inside the summation sign of Eq. (23) are symmetric with respect to $\eta_i = 0$, only N/2 terms are needed. However, the kernel that appears in Eq. (18) is not symmetric with respect to the variable of integration. Hence, it is still necessary to invert a N × N matrix even though only half of the vectors $P_k\left(\eta_i\right)$ are needed in Eq. (23). The inversion of a matrix with relatively large dimension generally requires an excessive amount of computing time. One way of minimizing the computing time required is to reduce the size of the matrix analytically beforehand. This can be done quite readily by partitioning the matrix $\mathbf{A}$ into four submatrices.

Assume the inverse $\mathbf{A}^{-1} = \mathbf{E}$. It is clear that

$$\mathbf{A}\mathbf{A}^{-1} = \begin{Bmatrix} A_{11}A_{12} \\ A_{21}A_{22} \end{Bmatrix} \begin{Bmatrix} E_{11}E_{12} \\ E_{21}E_{22} \end{Bmatrix} = \mathbf{I} \,, \tag{34}$$

where $\mathbf{I}$ is the identity matrix. Since the Gauss-Hermite weights and mesh points can be arranged in such a way that

$$A_{11} = A_{22} \tag{35}$$

$$A_{21} = A_{12} \tag{36}$$

it follows from Eq. (34) that

$$E_{11} = \left(A_{11} - A_{12}A_{11}^{-1}A_{12}\right)^{-1} \tag{37}$$

$$E_{12} = -A_{11}^{-1}A_{12}E_{22} \tag{38}$$

$$E_{22} = E_{11} \tag{39}$$

$$E_{21} = E_{12} \;. \tag{40}$$

Hence, in the actual numerical calculation, only two N/2 × N/2 matrix inversions are necessary instead of a N × N matrix. Since the computing time required for the matrix inversion approximately varies as the cube of the dimension N, a considerable saving in computing time may be achieved if the computing time for the additional matrix algebra in Eqs. (37) and (38) can be minimized. Once E_{11} and E_{12} are known, the vector $\mathbf{P}$ is simply

$$\mathbf{P} = \left(E_{11}E_{12}\right)\begin{pmatrix} B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \\ B_N \end{pmatrix} . \tag{41}$$

Further economization may be made on physical grounds. In the low-energy region where the average spacing becomes much larger than the Doppler width and the average natural width, $\omega(\xi)$ in Eq. (17) approaches a Dirac delta function and L_1 becomes

$$L_1 \underset{-}{\sim} \frac{1}{\langle D\rangle^2}\left\langle \Gamma_{xk} J\right\rangle_k \left\langle \frac{\Gamma_k}{2} J\right\rangle_k . \tag{41a}$$

The quantity K_1 vanishes. Similarly, the higher-order terms will also vanish. Hence, it is possible to set $K_n = 0$ whenever $\langle D\rangle/\Delta$ and $\langle D\rangle/\langle\Gamma\rangle$ become larger than certain values. The proposed method was found to be sufficiently fast that the latter condition for the limiting case is not needed.

V. ESTIMATION OF L_2

The second-order term L_2 can be estimated using the same technique discussed previously. Equation (11) can be written as

$$L_2 = -\frac{1}{2\langle D\rangle^2}\int_{-\infty}^{\infty}\sqrt{2\pi}\,\omega(\xi)\left\langle \Gamma_{xk}\left\{\sqrt{\pi/2}\,\frac{\exp\left[-(\Delta^2\xi^2/4)-\left(\Gamma_k|\xi|/2\right)\right]}{\beta_k} - P_k\left(\frac{\Gamma_k}{2}\,\xi\right)\right\}\right\rangle_k$$

$$\cdot\left\langle\frac{\Gamma_{k'}}{2}\,\sigma_p^{(eq)}\,\frac{d}{d\sigma_p^{(eq)}}P_{k'}\left(\frac{\Gamma_k}{2}\,\xi\right)\right\rangle_{k'}\,d\xi\ . \tag{42}$$

It is interesting to note that the only unknown in Eq. (42) is the quantity

$$\frac{d}{d\sigma_p^{(eq)}}\,P_k\left(\frac{\Gamma_k}{2}\,\xi\right)\ .$$

The latter quantity can be related to $P_k\left(\Gamma_k\xi/2\right)$. Let

$$R = -\,\sigma_p^{(eq)}\,\frac{\partial}{\partial\sigma_p^{(eq)}}\,P\left(\frac{\Gamma_k}{2}\,\xi\right)\ . \tag{43}$$

Differentiating Eq. (18) with respect to $\sigma_p^{(eq)}$ and replacing the integral by the Gauss-Hermite quadrature, one obtains a matrix equation of the form

$$\mathbf{A}\mathbf{R} = \mathbf{V}/N_0\ , \tag{44}$$

and

$$V_i = P_i\cdot\exp\left[\frac{\Delta^2\eta_i}{4\alpha^2}\right]\cdot\beta_k\ , \tag{44a}$$

where P_i is simply the solution of Eq. (26), and N_0 is the normalization factor defined by Eq. (28). Hence,

$$R = A^{-1}V/N_0 \,, \tag{45}$$

where A^{-1} has already been obtained in evaluating L_1. Thus, the second-order term can be obtained readily once the first-order term is known.

For the cases where the asymptotic formula is applicable, R is simply

$$R_k\left(\frac{\Gamma_k}{2}\,\xi\right) = \sqrt{\pi/2}\,\exp\left[-\frac{\Delta^2}{4}\,\xi^2 - \frac{\Gamma_k}{2}\,|\xi|\right]\left\{\frac{1 + 2\left[\rho - U_k(\xi)\right]\Big/\left(\beta_k + \rho\right)}{\left(\beta_k + \rho\right)^2}\right\}\cdot\beta_k \,, \tag{46}$$

where P_k and U are defined in Eq. (32) and Eq. (33a).

The same technique, in principle, can be extended to even higher-order terms. However, the evaluation of higher-order terms beyond the second order is believed to be unnecessary on physical grounds. For cases in the low-energy region where the self-shielding effect is large, the average spacing is generally much larger than the corresponding Doppler width and the natural width for all problems of practical interest. Under such conditions, all K_n terms vanish as $\omega(\xi)$ approaches the Dirac δ-function.

VI. CHOPSUEY CODE

In order to test and evaluate the merits of the proposed method, the CHOPSUEY code has been developed. The code uses the input and output routines of the RP-270 code written by Rago[11] with modifications to allow for both s- and p-wave resonances. Ten quadrature points were used for

both the neutron width and the fission width distributions. The fast J-integral routine developed recently[6] was incorporated. The statistical averaging and the calculation of the overlap terms are performed in the subroutine UNGRES and UNRES for the fissile and fertile isotopes, respectively. The effective cross sections for both s- and p-wave contributions are given separately in the output. In these subroutines, the average quantities $\left\langle \Gamma_x J \right\rangle$, $\left\langle \Gamma J \right\rangle$, $\left\langle \Gamma_x \int_0^\infty [\psi/(\beta + \psi)]^2 \, dx \right\rangle$ and $\left\langle \Gamma \int_0^\infty [\psi/(\beta + \psi)]^2 \, dx \right\rangle$ are calculated first. In the calculation of $P_k\left(\Gamma_k \xi_i/2\right)$, the code examines whether the k-*th* mesh point belongs to the asymptotic region or not. For the points that do not belong to the asymptotic region, a matrix inversion routine is called. The matrix inversion routine was written by Garbow[12] using the Jordan method. A FORTRAN listing of the relevant subroutines are listed in the Appendix.

One of the great concerns is whether the proposed method is efficient enough to be economical in routine applications. Test calculations have been made for problems with ^{239}Pu and ^{238}U using ENDF/B parameters. For fertile isotopes, computing time is generally negligible. The most severe test is believed to be the case when ^{239}Pu is in high concentration. In the calculation of ^{239}Pu cross sections, not only the averaging over the fission width distribution function is required, but also there are as many as 30 energy points for all five spin sequences. Two cases at room temperature were considered in the test calculations.

Case 1

$\underline{^{239}\text{Pu}}$: $\sigma_p^{(eq)} = 71.6/\text{atm}$

$\underline{^{238}\text{U}}$: $\sigma_p^{(eq)} = 40 \text{ b/atm}$

both the neutron width and the fission width distributions. The fast J-integral routine developed recently[5] was incorporated. The statistical averaging and the calculation of the overlap terms are performed in the subroutine UNRES and URES for the fissile and fertile isotopes, respectively. The effective cross sections for both s- and p-wave contributions are given separately in the output. In these subroutines, the average quantities $\left\langle \Gamma_x J\right\rangle$, $\langle \Gamma J\rangle$, $\left\langle \Gamma_x \int_0^\infty [\psi/(\xi + y)]^2\, dx\right\rangle$ and $\left\langle \Gamma \int_0^\infty [\psi/(\xi + x)]^2\, dx\right\rangle$ are calculated first. In the calculation of $P_k\left(\Gamma_k \xi_i/2\right)$, the code examines whether the k-th mesh point belongs to the asymptotic region or not. For the points that do not belong to the asymptotic region, a matrix inversion routine is called. The matrix inversion routine was written by Garbow[12] using the Jordan method. A FORTRAN listing of the relevant subroutines are listed in the Appendix.

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Case 1

^{239}Pu: $\sigma_p^{(eq)}$ = 71.6/atm

^{238}U: $\sigma_p^{(eq)}$ = 40 b/atm

Case 2

^{239}Pu: $\sigma_p^{(eq)} = 300$ b/atm

^{238}U: $\sigma_p^{(eq)} = 30$ b/atm

It should be noted that the calculations require much less time at higher temperatures as more entries to the asymptotic region become evident. Table I summarizes the results of the computer time required for the proposed method as compared to the time required for the old MC^2 routine[13] (Subroutine QFJ) without the overlap effect. The time estimates given in Table I include the input-output time as required by the CHOPSUEY code but exclude the compilation time and wait time.

From Table I, it is clear that the proposed method is much superior to the old subroutine not only on the theoretical ground but also in terms of the computing time. The significant improvement in the algorithm for evaluating the generalized J-integral discussed previously[6] is more than enough to compensate for the computing time required for the more rigorous treatment of the overlap effect.

TABLE I

Timing of CHOPSUEY

	sec
MC^2 (QFJ) (no overlap)	120
Proposed algorithms (overlap included)	
Case I	47
Case II	28

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APPENDIX

```
       SUBROUTINE UNGRES
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*4 T1,T2,T3,T4,TTO,TTJ,DD
      COMMON /QFJ1/ZETA,TOT2,BETA,PSIZ,PSIZ2,PS3
      COMMON/TRTI/TR(62,62),TI(62,62),AIMW,AX,REW,WHY,KI
      COMMON/H/TEST1,TEST2,HH
      COMMON/SEC/TOT3,TOT4
      COMMON/F/AKI,DEN,RAT,C,AAA
      COMMON/R/ EERFC,ARG
      COMMON/PP/ LL,LP,MU,NCS,IGEOM,NU,NOVLP
      COMMON/DP/ X,     E,GMNZ,G,T,UNR,AZERO,D,C4,ABAR,SIGPO,DZERO,
     1TITLE,   C3,CC,Y,UNRGM,UNRG,C1,C2,RAD,FLUXCT,CAP,FISS,SIGP
      DIMENSION X(10), E(100),UNR(100),TITLE(12),Y(10),UNRGM(100) ,
     1UNRG(100)                                                         DOP    8
      DIMENSION XXX(10),GN(10),GF(10)
      DIMENSION A(10,10),B(10,100),E1(20),E2(20),AVGGMT(20),AVGFMT(20) ,
     XAVGTMT(20),DUMMY(10,100),SI(20),E3(20),E4(20)
      DIMENSION FLUXCT(100),CAP(100),FISS(100)                          DOP    9
      DIMENSION YY(10),WW(10)                                           DOP   11
      DIMENSION GGF(100),GGM(100),TZETA(100),PPSIZ(100),H(100),GGFF(100)
     X,GGMM(100),BB(100),BBB(100)
      DIMENSION DUM1(5,10),DUM2(5,5),DUM3(5,5),DUM4(5,5),DUM6(5,5),
     XBP(10,1),VECT(10,1),DUM5(5,5),S(5,5)
      DIMENSION VECT2(10),DUMMY2(10,100),ANORM(10),BING(10),BINF(10),
     XBINT(10),AVT1(10)
      DIMENSION TTZETA(100)
      DATA  YY/3.436159118,2.532731674,1.756683649,1.036610829,
     X.3429013272,-3.436159118,-2.532731674,-1.756683649,-1.036610829,
     X-.3429013272/
      DATA WW/.7640432855D-5,.1343645746D-2,.3387439445D-1,.2401386110,
     X.6108626337,.7640432855D-5,.1343645746D-2,.3387439445D-1,.24013861
     X1,.6108626337/
      DATA E3/.1342138201D6,.6107756653D3,.2188797595D2,.2928709876D1,
     X.1124773092D1/
      DO 2 I=1,NCS                                                      DOP   32
      READ          100,SIGM1,SIGM2,GMGM,GMF
  100 FORMAT(5E12.5)                                                    DOP   34
      SIGP=C4+SIGM1+SIGM2                                               DOP   35
      GFBARJ=0.                                                         DOP   36
      BARJ=0.                                                           DOP   37
      TBARJ=0.0                                                         DOP   38
      TBARJ2=0.
      SEG=0.
      SEF=0.
      SET=0.
      FG=0.
      FF=0.                                                             DOP   76
      FT=0.                                                             DOP   77
      FG2=0.
      FF2=0.
      FT2=0.
      SRE=DSQRT(E(I))
      DELTIN=C3/SRE/2.                                                  DOP   40
      II=0
      JJ=0
      AVIND=0.
      AVINDF=0.
      AVINDT=0.
      AVO=0.
      T1=TLEFT(DD)
```

```
      DO 1 J=1,10                                                       DOP   41
      IF(LP.NE.0)GO TO 944                                              DOP   42
      GN(J)=GMNZ *SRE*X(J)
      GO TO 911                                                         DOP   44
  944 AAA=RAD*SRE/4.56D+2
      TMU=MU                                                            DOP   46
      V=TMU*AAA**2/(1.+AAA**2)                                          DOP   47
      IF(MU.GT.1)GO TO 999                                              DOP   48
      GN(J)=GMNZ *SRE*X(J)*V
      GO TO 911                                                         DOP   50
  999 XXX(1)=5.175533E-2                                                DOP   51
      XXX(2)=1.630645E-1                                                DOP   52
      XXX(3)=2.884221E-1                                                DOP   53
      XXX(4)=4.317743E-1                                                DOP   54
      XXX(5)=5.992178E-1                                                DOP   55
      XXX(6)=8.00573E-1                                                 DOP   56
      XXX(7)=1.053244                                                   DOP   57
      XXX(8)=1.393041                                                   DOP   58
      XXX(9)=1.916293                                                   DOP   59
      XXX(10)=3.302585                                                  DOP   60
      GN(J)=GMNZ *SRE*XXX(J)*V
  911 DO 1 K=1,10
      GF(K)=GMF*Y(K)                                                    DOP   63
      GAM=GN(J)+GF(K)+GAGM                                              DOP   64
      ZETA=GAM*DELTIN
      SIGZ=2.6E6*G*GN(J)/ E(I)/GAM
      BETA=SIGP/SIGZ                                                    DOP   67
      AVIND=AVIND+1./BETA
      AVINDF=AVINDF+GF(K)/BETA
      AVINDT=AVINDT+GAM/BETA
      AAAQ=GAM*DSQRT((BETA+1.)/BETA)
      AVQ=AVQ+AAAQ
      CALL FH
      FJF=TOT2
      FJF2=TOT3
      IF(NOVLP.NE.0.)GO TO 6
      TBARJ2=TBARJ2+FJF2*GAM
      TEST1=(BETA+PSIZ)/PSIZ
      IF(TEST1.GE.2.5)GO TO 5
      II=II+1
      BBB(II)=BETA
      GGFF(II)=GF(K)
      GGMM(II)=GAM
      TIZETA(II)=ZETA
      GO TO 6
    5 JJ=JJ+1
      BB(JJ)=BETA
      GGF(JJ)=GF(K)
      GGM(JJ)=GAM
      TZETA(JJ)=ZETA
      IF(TEST1.GE.4.5)GO TO 29
      ARG=.707106781*ZETA
      CALL RATNL
      PPSIZ(JJ)=.6266570686*ZETA*EERFC
      PSIZ2=PPSIZ(JJ)
   29 BPP=BETA+PSIZ2
      PPSIZ(JJ)=PSIZ2
      H(JJ)=BPP
    6 TBARJ=TBARJ+FJF*GAM
      BARJ=BARJ+FJF                                                     DOP   73
```

```
  1 GFBARJ=GFBARJ+FJF*GF(K)
    BARJ=.01*BARJ*GMGM/D
    GFBARJ=.01*GFBARJ/D
    TBARJ=.01*TBARJ/D
    IF(NOVLP.NE.0.)GO TO 709
    AVQ=.01*AVQ
    AVIND=.01570796327*AVIND*GMGM/D
    PRINT 730,AVIND,AVQ
730 FORMAT(7H AVIND=D12.5,5H AVQ=D12.5)
    AVGABB=AVQ
    PRINT 51,AVGABB
 51 FORMAT(8H AVGABB=D12.5)
    PRINT 8,II,JJ
  8 FORMAT(4H II=I6,4H JJ=I6)
    T2=TLEFT(DD)
    TIJ=(T1-T2)*.01
    T3=TLEFT(DD)
    BARING=AVIND
    BARINF=.01570796327*AVINDF/D
    BARINT=.01570796327*AVINDT/D
    TBARJ2=.01*TBARJ2/D
    D2=TBARJ2
    SEG=(BARING-BARJ)*D2
    SEF=(BARINF-GFBARJ)*D2
    SET=(BARINT-TBARJ)*D2
    PRINT 9151,SEG,SEF,SET,D2
9151 FORMAT(6E12.5)
    ALP=DSQRT(.5/DELTIN**2+(D*.318309)**2+AVGABB**2)
    DO 36 N=1,5
    SI(N)=DABS(YY(N)/ALP)
    ARG1=SI(N)
    E4(N)=DEXP(.5*(.5*ARG1/DELTIN)**2)
    E2(N)=E4(N)*E4(N)
    E1(N)=E3(N)/(E2(N)*E2(N))
    E1(N+5)=E1(N)
    E2(N+5)=E2(N)
    E3(N+5)=E3(N)
 36 CONTINUE
    IF(II.EQ.0)GO TO 7
    DO 33 J=1,II
    DO 11 N=1,5
    ARG1=SI(N)
    B(N,J)=1.2533156*DEXP(-.5*GGMM(J)*ARG1)
    ANORM(N)=E2(N)*(BBB(J)  +WW(N)*E3(N)*.25*GGMM(J)/ALP)
    BP(N,1)=B(N,J)/ANORM(N)
    BP(N+5,1)=BP(N,1)
    ANORM(N+5)=ANORM(N)
    DO 11 K=1,10
    IF(N.EQ.K)GO TO 110
    A(N,K)=.25*WW(K)*E1(K)*DEXP(.5*(1./DELTIN/ALP)**2*YY(N)*YY(K)-
   XDABS(YY(N)-YY(K))*.5*GGMM(J)/ALP)/ALP/ANORM(N)*E2(K)*GGMM(J)
    GO TO 111
110 A(N,K)=1.
111 IF(K.GT.5)GO TO 112
    S(N,K)=A(N,K)
    DUM5(N,K)=A(N,K)
    GO TO 11
112 DUM1(N,K-5)=A(N,K)
 11 CONTINUE
    CALL MATRIX(S,DETERM,5)
```

```
   DO 93 M=1,5
   DO 93 L=1,5
   DUM3(M,L)=0.
   DO 92 N=1,5
   DUM2(N,L)=0.
   DO 91 K=1,5
91 DUM2(N,L)=DUM2(N,L)+S(N,K)*DUM1(K,L)
92 DUM3(M,L)=DUM3(M,L)+DUM1(M,N)*DUM2(N,L)
   DUM4(M,L)=DUM5(M,L)-DUM3(M,L)
93 CONTINUE
   CALL MATRIX(DUM4,DETERM,5)
   DO 73 M=1,5
   VECT(M,1)=0.
   DO 75 N=1,10
   IF(N.GT.5)GO TO 74
   VECT(M,1)=VECT(M,1)+DUM4(M,N)*BP(N,1)
   DUM6(M,N)=0.
   DO 71 K=1,5
71 DUM6(M,N)=DUM6(M,N)+DUM2(M,K)*DUM4(K,N)
   DUM1(M,N+5)=-DUM6(M,N)
   GO TO 75
74 VECT(M,1)=VECT(M,1)+DUM1(M,N)*BP(N,1)
75 CONTINUE
   DUMMY(M,J)=VECT(M,1)
73 CONTINUE
   DO 76 M=1,5
   VECT2(M)=0.
   DO 77 N=1,10
   IF(N.GT.5)GO TO 78
   VECT2(M)=VECT2(M) +DUM4(M,N)*VECT(N,1)*E2(N)*BBB(J)/ANORM(N)
   GO TO 77
78 VECT2(M)=VECT2(M) +DUM1(M,N)*VECT(N-5,1)*E2(N)*BBB(J)/ANORM(N)
77 CONTINUE
   DUMMY2(M,J)=VECT2(M)
76 CONTINUE
33 CONTINUE
   DO 34 N=1,5
   AVGGMT(N)=0.
   AVGFMT(N)=0.
   AVGTMT(N)=0.
   AVT1(N)=0.
   BING(N)=0.
   BINF(N)=0.
   BINT(N)=0.
   DO 34 J=1,II
   AVGGMT(N)=AVGGMT(N)+DUMMY(N,J)*E2(N)
   AVGFMT(N)=AVGFMT(N)+DUMMY(N,J)*E2(N)*GGFF(J)
   AVGTMT(N)=AVGTMT(N)+DUMMY(N,J)*E2(N)*GGMM(J)
   BING(N)=BING(N)+B(N,J)/BBB(J)
   BINF(N)=BINF(N)+B(N,J)*GGFF(J)/BBB(J)
   BINT(N)=BINT(N)+B(N,J)*GGMM(J)/BBB(J)
   AVT1(N)=AVT1(N)+DUMMY2(N,J)*E2(N)*GGMM(J)
34 CONTINUE
 7 DO 3333 M=1,5
   AVGG=0.
   AVGF=0.
   AVGT=0.
   AVTQ2=0.
   AVGQ2=0.
   AVFQ2=0.
```

```
      [illegible]
      IF(JJ.EQ.0)GO TO 9
      ARG1=SI(M)
      QQ=D*ARG1/3.1416
      DUM=.5*ARG1/DELTIN/1.4142
      ARG=DUM
      CALL RATNL
      A1=E4(M)-EERFC
      Q=1.
      DO 333 J=1,JJ
      TEST6= H(J)/PPSIZ(J)
      IF(TEST6.GE.25.)GO TO 223
      ARG=DUM+TZETA(J)/1.4142
      CALL RATNL
      A2=EERFC
      U=.626658*TZETA(J)*(A1+A2)
      Q=1.+(PPSIZ(J)-U)/H(J)
      Q2=(H(J)/BB(J))-Q
      Q3=(Q-.5)*2.*BB(J)/H(J)
  223 EE1=DEXP(-.5*GGM(J)*ARG1)/H(J)
      AVGG=AVGG+EE1*Q
      AVGF=AVGF+GGF(J)*Q*EE1
      AVGT=AVGT+GGM(J)*Q*EE1
      IF(TEST6.GE.25.)GO TO 333
      AVGQ2=AVGQ2+Q2*EE1
      AVFQ2=AVFQ2+Q2*EE1*GGF(J)
      AVTQ2=AVTQ2+Q2*EE1*GGM(J)
      AVTQ3=AVTQ3+Q3*EE1*GGM(J)
  333 CONTINUE
      IF(II.GT.0)GO TO 9
      AVGGMT(M)=0.
      AVGFMT(M)=0.
      AVGTMT(M)=0.
      BING(M)=0.
      BINF(M)=0.
      BINT(M)=0.
      AVT1(M)=0.
    9 OVLG=.01*(AVGG+AVGGMT(M)*.7978836)*GMGM
      OVLF=.01*(AVGF+AVGFMT(M)*.7978836)
      OVLT=.01*(AVGT+AVGTMT(M)*.7978836)
      OVLG2=.01*(AVGQ2+ .7978836*(BING(M)-AVGGMT(M)))*GMGM
      OVLF2=.01*(AVFQ2+.7978836*(BINF(M)-AVGFMT(M)))
      OVLT2=.01*(AVTQ2+.7978836*(BINT(M)-AVGTMT(M)))
      OVLT3=.01*(AVTQ3+.7978836*AVT1(M))
  894 IF(QQ.GT.2.)GO TO 498
      FDYSON=(1.-QQ+.5*QQ*DLOG(1.+QQ))
      GO TO 933
  498 FDYSON=.5*QQ*DLOG((1.+QQ)/(QQ-1.))-1.
  933 DUM=WW(M)*OVLT*FDYSON*E1(M)*2./D
      FG=FG+OVLG*DUM
      FF=FF+OVLF*DUM
      FT=FT+OVLT*DUM
      DUMM=WW(M)*OVLT3*FDYSON*E1(M)*2./D
      FG2=FG2+DUMM*OVLG2
      FF2=FF2+DUMM*OVLF2
      FT2=FT2+DUMM*OVLT2
 3333 CONTINUE                                                              DOP
      OVERLG=(FG-FG2)*.3927/ALP
      OVERLF=(FF-FF2)*.3927/ALP
      OVERLT=(FT-FT2)*.3927/ALP
```

```
      DVG=BARJ*TBARJ-SEG-OVERLG
      DVF=GFBARJ*TBARJ-SEF-OVERLF
      DVT=TBARJ*TBARJ-SET-OVERLT
      PRINT 9151,FG,FG2,OVERLG,FF,FF2,OVERLF
      IF(DVG.GT.0.)GO TO 14
  709 DVG=0.
      DVF=0.
      DVT=0.
   14 PRINT 701,DVG,DVF,DVT
  701 FORMAT(5H DVG=D12.5,5H DVF=D12.5,5H DVT=D12.5)
      PRINT 702,BARJ,GFBARJ,TBARJ                                     DOP
  702 FORMAT(6H BARJ=E12.5,8H GFBARJ=E12.5,7H TBARJ=E12.5)            DOP
      UNRGM(I)=UNRGM(I)+SIGP*BARJ                                     DOP
      T4=TLEFT(DD)
      TTO=(T3-T4)*.01
      PRINT 13,TTJ,TTO
   13 FORMAT(5H TTJ=E12.5,5H TTO=E12.5)
      UNRG(I)=UNRG(I)+SIGP*GFBARJ                                     DOP
      FLUXCT(I)=1.-(TBARJ-DVT)
      CAP(I)=CAP(I)+SIGP*(BARJ-DVG)/FLUXCT(I)
      FISS(I)=FISS(I)+SIGP*(GFBARJ-DVF)/FLUXCT(I)
    2 CONTINUE                                                        DOP
      RETURN                                                          DOP
      END
      SUBROUTINE FH
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/TRTI/TR(62,62),TI(62,62),AIMW,AX,REW,WHY,KI
      COMMON/H/TEST1,TEST2,HH
      COMMON /QFJ1/ZETA.TOT2,BETA,PSIZ,PSIZ2,PS3
      COMMON/R/ EERFC,ARG
      COMMON/F/AKI,DEN,RAT,C,AAA
      COMMON/SEC/TOT3,TOT4
      DIMENSION ZLP(8)
      DIMENSION RAT(10),AKI(10),DEN(10)
      DIMENSION ALP(5)
      DIMENSION AN(10),BM(10)
      DATA AN/.1666667,.3333333D-1,.7142857D-2,.1587302D-2,
     X.3607504D-3,.8325008D-4/
      DATA BM/.1666667,.5555556D-1,.1234568D-1,.2057613D-2,
     X.2743484D-3,.3048316D-4/
      DATA ALP/.9848077530,.8660254038,.6427876097,.3420201433/
      DATA ZLP/     .2393156642,.4647231720,.6631226582,.8229838658,
     X.9350162426,.9927088740/
      KI=1
      WHY=.5*ZETA
      ARG=WHY
      CALL RAINL
      PSIZ=.8862269*ZETA*EERFC
      H=BETA+PSIZ
      TEST1=H/PSIZ
      AINTZ=.5/TEST1
      ASQ=AAA**2
      IF(TEST1.GE.15.)GO TO 100
      IF(ZETA.GT.2.5)GO TO 20
      IF(TEST1.GE.4.5)GO TO 100
      IF(BETA.GE..018)GO TO 2
      IF(ZETA.GE..5)GO TO 20
      BOVPSI=BETA/PSIZ
      IF(BOVPSI.GE..2)GO TO 2
      RB=4.*(1.8971+DLOG(1.+.7532929*ZETA/BETA))/ZETA**2
```

```
      TEST2=BB*BETA
      IF(TEST2.GT..03)GO TO 4
      GO TO 20
    2 C=5./ZETA
      GO TO 3
    4 IF(TEST2.LT.1.0)GO TO 11
      FAC=1.+.018*(BETA-.00128)/(BETA+.00128)+.08*BOVPSI
      C=.8292*DSQRT(BB)*FAC
      GO TO 3
   11 C=.7071*DSQRT(BB+(1.+BETA)/BETA)
    3 TOT2=0.
      TOT3=0.
      TOT4=0.
      DO 1 I=1,6
      AX=WHY*ZLP(I)*C/DSQRT(1.-ZLP(I)**2)
      CALL QUICKW
      PSI=.8862269*ZETA*REW
      AKI(I)=.8862269*ZETA*AIMW
      DEN(I)=BETA+PSI
      RAT(I)=PSI/DEN(I)/(1.-ZLP(I)**2)
      TOT3=TOT3+RAT(I)*BETA/DEN(I)
      AKISQ=AKI(I)**2*ASQ
      TOT4=TOT4+(AKISQ/(DEN(I)**2-AKISQ))*RAT(I)
    1 TOT2=TOT2+RAT(I)
      TOT2=TOT2+AINTZ
      TOT2=TOT2*C*.2416609733
      TOT3=TOT3+AINTZ*(1.-1./TEST1)
      TOT3=TOT3*C*.2416609733
      TOT4=TOT4*C*.2416609733
      RETURN
  100 ARG=.707106781*ZETA
      CALL RATNL
      PSIZ2=.6266570686*ZETA*EERFC
      HH=BETA+PSIZ2
      TOT2=1.57079632681/HH
      TOT3=TOT2*BETA/HH
      Z=ZETA*ZETA
      IF(ZETA.GT.2.5)GO TO 23
      ARG=.40824829*ZETA
      CALL RATNL
      PSIZ3=.7236021*ZETA*EERFC
      S=0.
      SUM=0.
      TEMP=1.
      DO 22 I=1,6
      TEMP=TEMP*Z
      SUM=SUM+BM(I)*TEMP
      S=S+AN(I)*(SUM+.25)
   22 CONTINUE
      S=S+.25
      ZEX=2.1708037*ZETA*DEXP(Z/6.)
      PS3=(PSIZ2*(3.*PSIZ3-ZEX)+1.5*Z*S)*1.5707963281
      GO TO 24
   23 TWOTHZ=.66666667*Z
      E1=(TWOTHZ*(TWOTHZ+2.334733)+.250621)/(TWOTHZ*(TWOTHZ+3.330657)+
     X1.681534)
      H1=1.-E1
      H2=1.5/Z-H1
      H3=5./(Z*Z)-1.1111111*H2
      H4=26.25/(Z*Z*Z)-1.1666667*H3
```

```
      PS3=.58904862*E1-(H1-H2+H3-H4)*.39269908
   24 TOT4=.3333333*ASQ*PS3/(HH*HH*HH)
      IF(TEST1.LT.15.)GO TO 33
      RETURN
   33 TOT2=TOT2+(PS3-PSIZ2*PSIZ2*1.5707963281)/(HH*HH*HH)
      TOT3=TOT3*(1.+3.*(.6366182837*PS3-PSIZ2*PSIZ2)/(HH*HH))
      TOT4=.3333333*ASQ*PS3/(HH*HH*HH)
      RETURN
   20 C=.7171*DSQRT((1.+BETA)/BETA)
      TOT2=0.
      TOT3=0.
      TOT4=0.
      DO 9 I=1,4
      AX=WHY*ALP(I)*C/DSQRT(1.-ALP(I)**2)
      CALL QUICKW
      PSI=.8862269*ZETA*REW
      AKI(I)=.8862269*ZETA*AIMW
      DEN(I)=BETA+PSI
      RAT(I)=PSI/DEN(I)/(1.-ALP(I)**2)
      TOT3=TOT3+RAT(I)*BETA/DEN(I)
      AKISQ=AKI(I)**2*ASQ
      TOT4=TOT4+(AKISQ/(DEN(I)**2-AKISQ))*RAT(I)
    9 TOT2=TOT2+RAT(I)
      TOT2=TOT2+AINTZ
      TOT2=TOT2*C*.3490658504
      TOT3=TOT3+AINTZ*(1.-1./TEST1)
      TOT3=TOT3*C*.3490658504
      TOT4=TOT4*C*.3490658504
      RETURN
      END
```